Computational Modeling of Chemical Reactions of Monomethylhydrazine and Nitrogen Dioxide: Molecular Dynamics and Wavepacket Dynamics

Yulun Han, Dane Hogoboom, Dmitri S. Kilin*

Department of Chemistry and Biochemistry, North Dakota State University, Fargo, North Dakota 58102

To accelerate the development of ideal hypergolic propellants, it is important to study chemical reactions precede ignition in the case of traditional hypergolic propellants. In this study, we adopt spin-unrestricted density functional theory (DFT) based molecular dynamics (MD) to investigate chemical reactions of a hypergolic mixture: monomethylhydrazine (CH_3NHNH_2) and nitrogen dioxide (NO_2). We observe three sequential steps of hydrogen transfer and other events such as the rupture of C-N bond. Energy diagrams related to hydrogen transfer reactions are constructed by post-processing the MD trajectory. The Bader charge analysis demonstrates the nature of hydrogen transfer processes is proton transfer rather than hydrogen abstraction. A wavepacket dynamics on the basis of ab initio potential energy surface (PES) obtained from the MD trajectory demonstrates quantum tunneling occurs under the reaction barrier.